Three-sublattice order in the SU(3) Heisenberg model

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Multi-Grid approach for matrix product states

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Challenges for numerics

Fermionic lattice models
• Phase diagrams of even simple models such as the $t$-$J$ or Hubbard model are still disputed

Frustrated spin systems
• Existence of exotic phases, in particular without local order as $T \to 0$
• Topological spin liquids
• Gapless spin liquids: Fermi sea of fractionalized excitations
• $SU(N)$ models, orbital models, Kondo models

Realistic systems
• Materials, quantum chemistry
• Structure factors of quasi-$1d$ frustrated magnets for neutron scattering
• Fraction Quantum Hall systems

Time evolution
• Equilibration/relaxation/thermalization
• Preparation of states in an optical lattice
Tensor networks in 2d

**PEPS, MERA, EPS, TTN, ...**
- Polynomial scaling for 2d systems, or even thermodynamic limit immediately
- Small bond dimension and little numerical experience

**The dark side: DMRG**
- DMRG scales exponentially in 2d!
- System sizes much larger than ED
- Several recent successes

Elegant, but somewhat uncontrolled

Brute force, but well-controlled

Maybe we should combine approaches?
Multi-flavor Hubbard models

- Multi-flavor Hubbard models can be realized in cold atomic gases

\[ H = -t \sum_{\langle i,j \rangle} \sum_{\alpha} \left( c_{i\alpha}^\dagger c_{j\alpha} + \text{h.c.} \right) + U \sum_i \sum_{\alpha \neq \beta} n_{i\alpha} n_{i\beta} \]

- Lots of cooling and commensurable filling: **Mott insulator**
- Even more cooling: **spin order**

**SU(2)**
- Square lattice: antiferromagnet
- Triangular lattice: 120° order

**SU(3)**
- Fix one particle per site
- Spin order unknown for both triangular and square lattice
SU(3) Heisenberg model

- We concentrate on three-flavor case with one particle per site and derive an effective model in $t/U$

$$H = J \sum_{\langle i,j \rangle} \sum_{\alpha,\beta} |\alpha_i \beta_j \rangle \langle \beta_i \alpha_j|$$

- We study the square and triangular lattice
Spin-$1$ bilinear-biquadratic model

$$H = \sum_{\langle i,j \rangle} \left[ \cos \theta (\vec{S}_i \cdot \vec{S}_j) + \sin \theta (\vec{S}_i \cdot \vec{S}_j)^2 \right]$$

- Mean-field phase diagram for the square lattice (Papanicolaou, 1988):
  - SU($3$) point at transition from antiferromagnet to “semi-ordered phase”
  - Square lattice does not give enough constraints to uniquely fix ordering in that phase
- Triangular lattice:
  - Enough constraints at the SU($3$) point: three-sublattice order
Mean-field phases

**Square lattice**
- Semi-ordered phase is characterized by infinitely many degenerate ground states between 2- and 3-sublattice order

**Triangular lattice**
- SU(3) point has three-sublattice order

Do quantum fluctuations select some type of order, or does a completely different phase emerge?
Previous work: Tóth et al, PRL 2010

Is this stable under quantum fluctuations?
The dark side: DMRG in 2d

- Review of recent work
- Choice of cluster size and boundary conditions
- Measurements
- Results
Some recent 2d DMRG results

- **White & Chernyshev, PRL 99, 127004 (2007)**
  - SU(2) Heisenberg model on square and triangular lattice
  - Results for square lattice with similar accuracy as MC after careful extrapolation in truncated weight and system size
  - Lots of prior knowledge from spin-wave theory
Some recent 2d DMRG results

- **Yan, Huse & White, Science 332, 6034 (2011)**
  - Spin liquid ground state on the Kagome lattice
  - Previous best energy: Evenbly & Vidal, PRL 104, 187203 (2010)
  - See also Stefan Depenbrock’s poster downstairs

- **Jiang,Yao & Balents 2011, arXiv:1112.2241**
  - Spin liquid ground state in the $J_1$-$J_2$ model on the square lattice
  - Previous work with PEPS: Murg, Verstraete & Cirac, PRB 79, 195119 (2009)
Some recent 2d DMRG results

- Jiang, Gu, Qi & Trebst, PRB 83, 245104 (2011)
  - Heisenberg-Kitaev model with magnetic field
  - Interpolates between Kitaev’s honeycomb model and Heisenberg model and describes certain Iridate compounds

![Phase diagram](image)

For the magnetically ordered states we find that the orientation of the magnetic field $\alpha$ perturbation theory reveals a rich sequence of three phases. For sufficiently large magnetic field, the order of both Neel AFM and stripy AFM are destroyed and they give way to a simple polarized phase. Including a magnetic field, the transition between the polarized state and these canted phases is destroyed and they give way to a simple polarized phase. Our numerical simulations strongly suggest that the gapless excitations of this phase are emergent Majorana modes.

The phase diagram evolves out of this sequence of three phases. Approaching the endpoint of a three-fold rotation around an arbitrary lattice site and a reflection symmetry, there is an additional simultaneous symmetry breaking. On the other hand, the transition from the polarized state to the canted phases is continuous, which is in agreement with their spontaneous symmetry breakings. The canted stripy phase breaks both of the two discrete symmetries of a three-fold rotation around an arbitrary lattice site and a reflection symmetry, which thus leads to a six-fold groundstate degeneracy in this phase. The canted stripy phase breaks a subset of these discrete symmetries of the energy gap.

For the magnetically ordered states we find that the orientation of the magnetic field $\alpha$, which is found across this transition – as shown in Fig1. For increasing $\alpha$, there is an additional simultaneous symmetry breaking. The canted stripy phase breaks a subset of these discrete symmetries of a three-fold rotation around an arbitrary lattice site and a reflection symmetry, which thus leads to a six-fold groundstate degeneracy in this phase. The canted stripy phase breaks a subset of these discrete symmetries of a three-fold rotation around an arbitrary lattice site and a reflection symmetry, which thus leads to a six-fold groundstate degeneracy in this phase. The canted stripy phase breaks a subset of these discrete symmetries of a three-fold rotation around an arbitrary lattice site and a reflection symmetry, which thus leads to a six-fold groundstate degeneracy in this phase.

The phase diagram shown in Fig 1 by first recapitulating previous extensive scans of the groundstate energy and magnetization effects. We have determined the phase boundaries in Fig 1 by giving excellent convergence with typical truncation errors but one also has to work with complex data types due to the lack of SUx invariance. It should be noted that the numerical analysis of Hamiltonian spanning by multiples of a generic Hamiltonian leads to a polarized state.
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DMRG in $2d$: entanglement

- Bond dimension of the MPS:
  \[ M \sim \exp S \]

- Scaling of entanglement:
  \[ S \sim W \]
  \[ S \sim L \]

- There is an easy (L) and a hard (W) direction!

Use long rectangles!
DMRG in 2d: boundaries

- Physically, periodic boundary conditions are often preferable
- In 1d DMRG: $S \rightarrow 2S$
  - Naive approaches need the square of the bond dimension, better approaches exist but numerically not as robust and precise
- PBC in 2d DMRG:
  - $L$ direction: same problem as 1d
  - $W$ direction: not as bad
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Use cylinders, avoid the torus!
Scaling

MPO bond dimension: $D \sim W$

Computation: $O(LW \cdot D \cdot M^3) + O(LW \cdot D^2 \cdot M^2)$

Memory: $O(D \cdot M^2)$

Disk: $O(LW \cdot D \cdot M^2)$

Without SU(2) symmetry: memory and disk space are limiting factors!
DMRG in 2d: local moments

- Long-range correlations are not reliable for 2d systems
- Break symmetries by hand at the boundary and watch the system far away!
- Reduces entanglement significantly

“Pinned” order with flavor-dependent chemical potential
DMRG in 2d: extrapolation

- Long-standing question: *what’s the correct way to extrapolate?*
  - **Number of states**: usually not very reliable
  - **Truncated weight**: standard technique, but sometimes difficult with single-site update
  - **Energy variance**: computationally difficult for large 2d system and complex Hamiltonians
The dark side: DMRG in 2d

- Review of recent work
- Measurements
- Choice of cluster size and boundary conditions
- Results
iPEPS

- Square lattice ansatz for both square and triangular lattice: *P. Corboz et al, PRB 82, 45119 (2010)*
- Directional corner transfer matrix scheme for general unit cells: *P. Corboz et al, PRB 84, 041108 (2011)*
  - 3x3 unit cell to stabilize three-sublattice state, 2x2 unit cell for antiferromagnet
- $Z_3$ symmetry: *Bauer et al, PRB 83, 125106 (2011)*
DMRG results

• Unknown finite-size scaling: stick to (almost) square systems

• Computational challenges:
  • Large dimension of the MPO (~twice of SU(2) case)
  • Need to use large bond dimension already in early stages due to non-mean field nature of the order
  • Very large entanglement

• Up to $M \sim 5000$ states, check for up to $M \sim 6400$ in some cases → system size up to 8x8
DMRG results

6x8 square lattice, cylindrical BCs, $M=4800$

Huge finite-size corrections for periodic chain → use open boundaries after all
DMRG results

\[ \langle m \rangle \]

\[ x \]

- 1, 2, 3, 4, 5, 6, 7, 8, 9

- y=2, y=3, y=4, y=5, y=6
Triangular lattice

- Energies of all methods match qualitatively
- iPEPS 3x3 is much lower than iPEPS 2x2
- DMRG has weak finite-size dependence

- Order parameters are consistent with 40-50 % of saturation moment
Square lattice

- Again, iPEPS 3x3 has much lower energy than iPEPS 2x2
- DMRG energies are comparable and consistent with ED

- Strong dependence of moment in iPEPS calculation leaves a large margin of error
- DMRG results seem consistent with magnetization in the range 30-40% of the saturation moment
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Systems with various scales

- Local optimization (DMRG) *almost* always works
- One class of exceptions: *dilute systems*
  - Weakly doped systems (cf. Davide Rossini’s talk last Monday)
  - Discretized continuous systems
- These systems have various length scales:
  - Doped systems: lattice spacing, size of a hole, global density modulation
  - Discretized continuous systems: discretization $dx$, external potential
- Energy scales: hopping $\sim 1/dx^2$, interaction $\sim 1/dx$, potential $\sim 1$
Multi-grid approaches

- Standard method for partial differential equations: solve the system on different length scales

Coarse grid
Global properties

Intermediate grids

Fine grid
Local properties

- Example: bosons with contact interaction in a shallow optical lattice
Multi-grid & MPS

Restriction:

Prolongation:

SVD
Multi-grid & MPS

- Construct Hamiltonian for several discretizations
- Start on coarse grid
- Perform DMRG
- Prolongate state
- Restrict state
- Perform DMRG
MG-DMRG: results

- Convergence often much more reliable than standard DMRG approaches
- Key difference to tree tensor network: the final result is only an MPS on one layer
- Extension to lattice models: how to construct Hamiltonians for coarser lattice?
  - CORE? Applying isometries to the MPO?
Conclusion

• Convincing numerical evidence for three-sublattice order on both the square and the triangular lattice

• Completely different ordering mechanisms:
  • Unique order at mean-field level on triangular lattice
  • Quantum fluctuations select the three-sublattice order over other states on the square lattice

• Combination of two tensor-network states builds more trust in results

• Both iPEPS and 2d DMRG are valuable tools for understanding 2d systems

• MG-DMRG provides a way to converge MPS ground states reliably when system has various length scales